An Integrated Approach to Modeling and Mitigating SOFC Failure
(Agreement No. DE-AC26-02NT41571)

Monthly Project Highlight Report

for the period of

October 1, 2002 – October 31, 2002

to

Dr. Don Collins
National Energy Technology Laboratory

From

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October 30, 2002

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Summary of Activities

The project officially started on October 1, 2002. Major activities of this month include

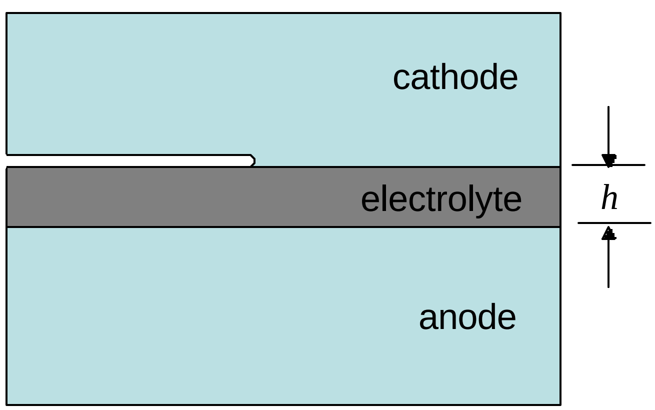
* In consultation with NETL program manager, we have finalized the statement of work for the Phase I project.
* Two graduate students have been hired to work on the project. One of them will focus on fracture mechanics, the other will focus on thermal shock related issues.
* A postdoc is being hire, who will be focusing on thermal/fluid and electrochemical tasks.
* Georgia Tech team has been meeting bi-weakly to discuss progresses and concerns.
* Two Georgia Tech team members attended the project kick-off meeting.
* Two telephone conferences were held with NETL project manager and simulation team.

Technical Highlights

Task 1: Fracture Mechanics Modeling

Task 1.1 Obtain fracture mechanics parameters for cohesive, interfacial and impinging cracks.

This month, we have focused on the delamination crack in the basic cathode-electrolyte-anode cell structure as shown in the figure below.



By assuming that the thickness of the electrolyte layer is much less than the thickness of the electrodes, we found that the stress intensity factor at the delamination crack tip is given by

$$K = h^{-i\epsilon}\left(\frac{1-\alpha}{1-\beta^2}\right)^{\frac{1}{2}}(K_I + iK_{II})\exp(i\omega)$$

and the corresponding energy release rate is

$$G = \frac{1-b^2}{E_*}|K|^2$$

In the above expressions, the variables a, b, w and E_* are related to the elastic modulus of the materials [Qu, J. and Bassani, J.L., "Fracture Mechanics of Interface Cracks in Anisotropic Materials," *J. Appl. Mech*., 60, p.422 - 431, 1993], and K_I and K_{II} are related to the temperature induced stress fields and the thickness of the electrodes. Based on dimensional analysis, we have

$$K_I^2 + K_{II}^2 = \Delta T \Delta a E K$$

where ΔT is the temperature change, Δa is the thermal mismatch between the cell materials, E is the Young's modulus of the electrolyte, and K is a function of the geometry and properties. In general, K must be obtained using numerical methods, such as the finite element method.

Based on the available data in the open literature, approximate values of the elastic constants for the cell materials are listed in the following table.

Materials	Young's modulus (GPa)	Poisson's ratio	CTE (10-6/^{o}C)
Cathode (LSM + YSZ)	90	0.3	11
Electrolyte (YSZ)	200	0.3	13
Anode (Ni + YSZ)	96	0.3	11

Based on these values, we have

$$a = -0.38 \;,\; b = -0.19 \;,\; w = 3.4 \;,\; E_* = 136 \text{ GPa}$$

Thus, the corresponding energy release rate is given by

$$G = 2.8 \Delta T K$$

Note that the energy release rate is a function of the phase angle w. The above value is for $w = 3.4$.

To assess the propensity of delamination fracture, the energy release rate should be compared with the interfacial fracture toughness, G_c , i.e.,

$$G = 2.8 \Delta T K \le G_c \, .$$

Once the function K is evaluated based on the temperature-induced stress fields, the above equation can be use to determining whether a delamination crack can propagate under given temperature change.

Task 2: Electrochemical Modeling

Task 2.1: Utilize/adapt existing electrochemical models, and develop enhancements necessary to achieve the project objectives and to advance the state-of-the-art

We have conducted and will continue a thorough literature search and methodology formulation for utilizing a more rigorous electrochemical governing equation for current density calculation as a function of cell operating voltage. A key reference thus far is the work by Kim et al. [Journal of the Electrochemical Society, 146(1), pp. 69-78, 1999]. This paper was cited by the PNNL fuel cell modeling group, and it focuses upon modeling anode-supported, planar SOFCs. Along with this reference, the "slice technique" modeling approach underlying Haynes' previous successes in simulating the Siemens Westinghouse tubular design are being leveraged into an imminent model of planar SOFCs.

Task 2.2: Models Extension to include porous electrode phenomena enhancements beyond the current state-of-the-art

The referenced paper by Kim et al. includes the concepts of ohmic charge transfer resistance, effective charge transfer resistance, and permeation factors as functions of electrode dimensions and topology. These concepts will enhance polarization simulation for porous SOFC electrodes, and will be added to the model under development.

Task 3: Thermal Modeling

Following extensive discussions with the NETL project management and modeling team (Conference call with Dr. Collins and Rogers on Tuesday, Oct. 29, 2002), the focus of the Georgia Tech team efforts should be on accurate treatment of heat transfer in the stack and including thermal radiation in the model for accurate predictions, especially in the situation when significant temperature gradients may be present in the cell (e.g., cold start-up and presence of the "hot" external reforming box between the cells). Other areas of emphasis are development of effective mass diffusivity models and thermal conductivity of the porous regions.

Task 3.1: Formulation of 2-D and 3-D models for combined advection, conduction, and radiation heat and mass transfer in the porous electrodes

A preliminary approach to thermal-fluid modeling of SOFC has been formulated and presented to the SECA team members and industrial partners at the SECA Modeling and Simulation Team – Integration Meeting on October 15, 2002.

Task 3.2: Formulation of an approach for calculation of effective transport, thermophysical and radiative properties for the porous electrodes

An accurate modeling of radiative heat transfer in the SOFC components was identified as the point of research focus for immediate efforts. Preliminary optical data for the ceramic materials (Y_2O_3 and MnO) that are similar to the materials used in SOFC have been identified and used to assess the optical thickness of the SOFC components. The ultimate goal of this effort is to select a proper approach for computing effective radiative properties of the SOFC materials and to identify a proper modeling strategy for computing radiative heat transfer.

Task 4: Multi-physics model integration

Task 4.1: Review the implementation strategy of developed modeling modules within the PNNL/NETL simulation platform

Initial communications between PNNL/NETL and the team have been accomplished. Specifically, both labs provided an overview of their methodologies at the October 15 kick-off meeting, and a follow-up conference call meeting was held with the NETL team and FLUENT representatives. A key result of this latter accomplishment was NETL's agreement to provide representative FLUENT files for the Georgia Tech team to further familiarize itself with the simulation code already synthesized.

Based on the discussions with NETL project management and modeling team, it is decided that the multi-physics integration should be accomplished by including modeling modules/subroutine for simulation of radiative heat transfer, effective thermal conductivity, and mass diffusivity (developed by Georgia Tech team) into the Fluent-based SOFC stack that is being developed by NETL team.

Completed Tasks

All tasks are on going.

Key Milestone Update

The team has become tangibly partnered with the NETL modeling group, led by Bill Rogers. This facilitates the envisioned collaboration between Georgia Tech and SECA lab partners.

Discussion Topics

One of the Georgia Tech's Co-PI, Dr. Andrei Fedorov, is not a US citizen. This has prevented him from attending the project kick-off meeting. As a result, our presentation on the thermal tasks was affected. It is hoped that the paper work be processed by DOE soon so that Dr. Fedorov will be able to attend the next meeting or site visit to other national labs.

Significant Accomplishments

No results to report for this reporting period.

Science & Technology Transfer

No science and technology transfer activities to report for this reporting period.

Presentations & Publications

Our research team made a presentation at the SECA Modeling and Simulation Team – Integration Meeting on October 15, 2002.

Site Visits

A trip to visit ORNL is planned. The purpose of the visit is to discuss material characterization issues with Dr. Edgar Lara-Curzio of ORNL.

Travel

Drs. Jianmin Qu and Comas Haynes traveled to Pittsburg on October 15, 2002 to attend the SECA Modeling and Simulation Team – Integration Meeting. A presentation was made at the meeting to outline our research objectives and approaches.